

Quantum discord for two-qubit CS states: Analytical solution

M A Yurishchev*

Institute of Problems of Chemical Physics of the Russian Academy of Sciences,

142432 Chernogolovka, Moscow Region, Russia

Abstract

We found an universal *local* orthogonal transformation which transforms any centrosymmetric (CS) density matrix ρ_{CS} into the X density matrix ρ_X : $H \otimes H \rho_{CS} H \otimes H = \rho_X$, where H is the Hadamard transformation. Since quantum discord is invariant under the local unitary transformations, this remarkable property allows to get the discord of general two-qubit CS states in an analytical form using the corresponding well-known formulas for the X states. Examples of systems with the CS density matrices are given, including XXZ spin model with the Dzyaloshinsky-Moriya interaction, a gas of spin-carrying particles in closed nanopore, and a family of pseudopure states.

PACS numbers: 03.65.Ud, 03.67.-a, 75.10.Jm

*Electronic address: yur@itp.ac.ru

Introduction. Quantum discord, Q , is a more general measure of quantum correlation than entanglement. Discord is important in quantum information theory, quantum metrology, condensed matter physics, and so on [1]. The evaluation of discord is a very hard problem. Even for two-qubit systems, the analytical calculations are restricted to the so-called X states. The term “X states” has been introduced in 2007 [2] and denotes the 4×4 density matrices which may have non-zero entries only along the main diagonal and anti-diagonal. Algebraic properties of such matrices were studied by Rau [3]. Analytical solution for the quantum discord of X density matrices has been obtained in Ref. [4]. On the other hand, there is a number of physical systems for which the density matrices have different forms, e. g., centrosymmetric ones. The $n \times n$ CS matrix is defined by the relations for its elements: $a_{ij} = a_{n-i+1, n-j+1}$ (about the CS matrices see, for example, the reviews [5] and references therein). In this communication we establish a connection between CS and X matrices through the local orthogonal transformation. Thanks to the fact [1] that the discord (and the entanglement) does not change its value under such transformations, we as a result obtain a possibility for the analytic calculation of discord in arbitrary two-qubit CS states.

CS and X matrices. In quantum mechanics the density matrix must be Hermitian, non-negativity defined, and have unit trace. A general 4×4 CS density matrix can be written as

$$\rho_{CS} = \begin{pmatrix} p_1 & p_2 + ip_3 & p_4 + ip_5 & p_6 \\ p_2 - ip_3 & \frac{1}{2} - p_1 & p_7 & p_4 - ip_5 \\ p_4 - ip_5 & p_7 & \frac{1}{2} - p_1 & p_2 - ip_3 \\ p_6 & p_4 + ip_5 & p_2 + ip_3 & p_1 \end{pmatrix}. \quad (1)$$

It contains seven real parameters p_1, \dots, p_7 . For the X state we have

$$\rho_X = \begin{pmatrix} \rho_{11} & 0 & 0 & \rho_{14} \\ 0 & \rho_{22} & \rho_{23} & 0 \\ 0 & \rho_{32} & \rho_{33} & 0 \\ \rho_{41} & 0 & 0 & \rho_{44} \end{pmatrix} = \begin{pmatrix} q_1 & 0 & 0 & q_4 + iq_5 \\ 0 & q_2 & q_6 + iq_7 & 0 \\ 0 & q_6 - iq_7 & q_3 & 0 \\ q_4 - iq_5 & 0 & 0 & 1 - q_1 - q_2 - q_3 \end{pmatrix}. \quad (2)$$

This matrix has also seven real parameters q_1, \dots, q_7 . Let us consider the transformation

$$R = H \otimes H = \frac{1}{2} \begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & -1 & 1 & -1 \\ 1 & 1 & -1 & -1 \\ 1 & -1 & -1 & 1 \end{pmatrix}, \quad (3)$$

where

$$H = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \quad (4)$$

is the Hadamard transform. The matrix R is orthogonal and $R^T = R$ (the superscript T denotes a transposition). Taking the matrices (1)–(3) and performing straightforward calculations we establish the following relations

$$H \otimes H \rho_{CS} H \otimes H = \rho_X \quad (5)$$

and

$$H \otimes H \rho_X H \otimes H = \rho_{CS}. \quad (6)$$

Here the parameters of both matrices are related as

$$\begin{aligned} \rho_{11} = q_1 &= \frac{1}{4} + p_2 + p_4 + \frac{1}{2}(p_6 + p_7), \\ \rho_{22} = q_2 &= \frac{1}{4} - p_2 + p_4 - \frac{1}{2}(p_6 + p_7), \\ \rho_{33} = q_3 &= \frac{1}{4} + p_2 - p_4 - \frac{1}{2}(p_6 + p_7), \\ \rho_{44} = 1 - q_1 - q_2 - q_3 &= \frac{1}{4} - p_2 - p_4 + \frac{1}{2}(p_6 + p_7), \\ \text{Re}\rho_{14} = \text{Re}\rho_{41} = q_4 &= -\frac{1}{4} + p_1 + \frac{1}{2}(p_6 - p_7), \\ \text{Im}\rho_{14} = -\text{Im}\rho_{41} = q_5 &= -p_3 - p_5, \\ \text{Re}\rho_{23} = \text{Re}\rho_{32} = q_6 &= -\frac{1}{4} + p_1 - \frac{1}{2}(p_6 - p_7), \\ \text{Im}\rho_{23} = -\text{Im}\rho_{32} = q_7 &= p_3 - p_5 \end{aligned} \quad (7)$$

and, vice versa,

$$\begin{aligned} p_1 &= \frac{1}{4} + \frac{1}{2}(q_4 + q_6), \\ p_2 &= -\frac{1}{4} + \frac{1}{2}(q_1 + q_3), \\ p_3 &= -\frac{1}{2}(q_5 - q_7), \\ p_4 &= -\frac{1}{4} + \frac{1}{2}(q_1 + q_2), \\ p_5 &= -\frac{1}{2}(q_5 + q_7), \\ p_6 &= \frac{1}{4} - \frac{1}{2}(q_2 + q_3 - q_4 + q_6), \\ p_7 &= \frac{1}{4} - \frac{1}{2}(q_2 + q_3 + q_4 - q_6). \end{aligned} \quad (8)$$

It is easy to proof the same using the Bloch forms for the density matrices ρ_{CS} and ρ_X . Indeed, expanding the density matrix (1) on the Pauli matrices one obtains

$$\begin{aligned}\rho_{CS} = & \frac{1}{4}[1 + 4p_4\sigma_x \otimes 1 + 4p_21 \otimes \sigma_x + 2(p_6 + p_7)\sigma_x \otimes \sigma_x + 2(p_7 - p_6)\sigma_y \otimes \sigma_y \\ & + (4p_1 - 1)\sigma_z \otimes \sigma_z - 4p_3\sigma_z \otimes \sigma_y - 4p_5\sigma_y \otimes \sigma_z].\end{aligned}\quad (9)$$

Performing the Hadamard transformations and taking into account that $H\sigma_x H = \sigma_z$, $H\sigma_y H = -\sigma_y$, and $H\sigma_z H = \sigma_x$, we obtain

$$\begin{aligned}H \otimes H \rho_{CS} H \otimes H = & \frac{1}{4}[1 + 4p_4\sigma_z \otimes 1 + 4p_21 \otimes \sigma_z + 2(p_6 + p_7)\sigma_z \otimes \sigma_z + 2(p_7 - p_6)\sigma_y \otimes \sigma_y \\ & + (4p_1 - 1)\sigma_x \otimes \sigma_x + 4p_3\sigma_x \otimes \sigma_y + 4p_5\sigma_y \otimes \sigma_x] = \rho_X.\end{aligned}\quad (10)$$

The last equality follows from the Bloch form for the matrix (2)

$$\begin{aligned}\rho_X = & \frac{1}{4}\{1 - [1 - 2(q_1 + q_2)]\sigma_z \otimes 1 - [1 - 2(q_1 + q_3)]1 \otimes \sigma_z + 2(q_4 + q_6)\sigma_x \otimes \sigma_x \\ & + 2(q_6 - q_4)\sigma_y \otimes \sigma_y + [1 - 2(q_2 + q_3)]\sigma_z \otimes \sigma_z - 2(q_5 - q_7)\sigma_x \otimes \sigma_y \\ & - 2(q_5 + q_7)\sigma_y \otimes \sigma_x\}\end{aligned}\quad (11)$$

and the relations (7).

As a result, we conclude that the quantum discord of the state ρ_{CS} is expressed through the discord of the state ρ_X :

$$Q(\rho_{CS}) = Q(\rho_X), \quad (12)$$

where the entries of ρ_X are given by Eqs. (7). Together with the analytical formulas for the discord of X states [4], this completes our solution.

Physical examples. As a first illustration, consider the anisotropic XXZ model with the Dzyaloshinsky-Moriya interaction. When the Dzyaloshinsky vector \mathbf{D} is oriented along x -direction, the Hamiltonian for the two-qubit chain reads [6]

$$\mathcal{H} = J\sigma_1^x\sigma_2^x + J\sigma_1^y\sigma_2^y + J_z\sigma_1^z\sigma_2^z + D_x(\sigma_1^y\sigma_2^z - \sigma_1^z\sigma_2^y). \quad (13)$$

Here J and J_z are the coupling constants and σ_i^α ($i = 1, 2$ and $\alpha = x, y, z$) are the Pauli matrices. In open form the Hamiltonian is given as

$$\mathcal{H} = \begin{pmatrix} J_z & iD_x & -iD_x & 0 \\ -iD_x & -J_z & 2J & iD_x \\ iD_x & 2J & -J_z & -iD_x \\ 0 & -iD_x & iD_x & J_z \end{pmatrix}. \quad (14)$$

This matrix is centrosymmetric. Because the sums and products of CS matrices are again the CS matrix, the corresponding Gibbs density matrix is CS one. Therefore, the thermal quantum discord is found here in an exact analytical form.

Another example is related to the dynamics in NMR of quantum correlation (discord) for the pair of nuclear spins in a nanopore filled with a gas of spin-carrying molecules or atoms [7]. The corresponding reduced density matrix is also the CS one:

$$\rho = \begin{pmatrix} \frac{1}{4} & \frac{1}{2}p - iu & \frac{1}{2}p - iu & q - r \\ \frac{1}{2}p + iu & \frac{1}{4} & q + r & \frac{1}{2}p + iu \\ \frac{1}{2}p + iu & q + r & \frac{1}{4} & \frac{1}{2}p + iu \\ q - r & \frac{1}{2}p - iu & \frac{1}{2}p - iu & \frac{1}{4} \end{pmatrix}, \quad (15)$$

where the correlation functions equal

$$\begin{aligned} p &= \frac{1}{2} \tanh \frac{\beta}{2} \cos^{N-1}(at), \\ q &= \frac{1}{8} \tanh^2 \frac{\beta}{2} [1 + \cos^{N-2}(2at)], \\ r &= \frac{1}{8} \tanh^2 \frac{\beta}{2} [1 - \cos^{N-2}(2at)], \\ u &= \frac{1}{4} \tanh \frac{\beta}{2} \cos^{N-2}(at) \sin(at). \end{aligned} \quad (16)$$

In these relations, N is the number of particles confined in a nanopore, a is the normalized coupling constant, and β is the inverse dimensionless temperature. In the paper [7], it was succeeded to calculate the quantum discord only for a particular case $p = u = 0$ and $q = r$ when the density matrix (15) is reduced to the Bell-diagonal form. Applying the method developed above we see that after performing the Hadamard transformation (5), the matrix (15) takes the X structure

$$\rho' = \begin{pmatrix} \frac{1}{4} + p + q & 0 & 0 & -r + 2iu \\ 0 & \frac{1}{4} - q & r & 0 \\ 0 & r & \frac{1}{4} - q & 0 \\ -r - 2iu & 0 & 0 & \frac{1}{4} - p + q \end{pmatrix}, \quad (17)$$

or in the Bloch form:

$$\rho' = \frac{1}{4} [1 + 2p(\sigma_1^z + \sigma_2^z) + 4r\sigma_1^y\sigma_2^y + 4q\sigma_1^z\sigma_2^z - u(\sigma_1^x\sigma_2^y + \sigma_1^y\sigma_2^x)]. \quad (18)$$

Using the general formulas of Ref. 4 we can in principle get the discord. But there is a simpler way. Indeed, perform an additional local unitary transformation to eliminate ‘ xy ’ cross-terms in Eq. (18), that is to reduce the density matrix (17) to the *real* X form. We are achieving this goal with the transformation $U \otimes U \rho' U^\dagger \otimes U^\dagger \equiv \rho''$, where $U = \exp(-i\varphi\sigma_z/2)$ and $\varphi = -\frac{1}{2} \arctan(2u/r)$. After this transformation, the density matrix (17) takes the form

$$\rho'' = \begin{pmatrix} \frac{1}{4} + p + q & 0 & 0 & 2u \sin 2\varphi - r \cos 2\varphi \\ 0 & \frac{1}{4} - q & r & 0 \\ 0 & r & \frac{1}{4} - q & 0 \\ 2u \sin 2\varphi - r \cos 2\varphi & 0 & 0 & \frac{1}{4} - p + q \end{pmatrix}, \quad (19)$$

that is

$$\begin{aligned} \rho'' = & \frac{1}{4} [1 + 2p(\sigma_1^z + \sigma_2^z) + 4(r \sin^2 \varphi + u \sin 2\varphi)\sigma_1^x \sigma_2^x + 4(r \cos^2 \varphi - u \sin 2\varphi)\sigma_1^y \sigma_2^y \\ & + 4q\sigma_1^z \sigma_2^z]. \end{aligned} \quad (20)$$

Using now the formulas for calculating the quantum discord for the real X density matrices [8] we finally obtain

$$Q = \min\{Q_1, Q_2\}, \quad (21)$$

where

$$\begin{aligned} Q_1 = & S_r - S - \left(\frac{1}{4} + p + q\right) \log_2 \frac{\frac{1}{4} + p + q}{\frac{1}{2} + p} - \left(\frac{1}{4} - q\right) \log_2 \frac{\frac{1}{4} - q}{\frac{1}{2} + p} \\ & - \left(\frac{1}{4} - p + q\right) \log_2 \frac{\frac{1}{4} - p + q}{\frac{1}{2} - p} - \left(\frac{1}{4} - q\right) \log_2 \frac{\frac{1}{4} - q}{\frac{1}{2} - p}, \end{aligned} \quad (22)$$

$$Q_2 = S_r - S - D_1 \log_2 D_1 - D_2 \log_2 D_2, \quad (23)$$

and

$$D_{1,2} = \frac{1}{2} \llbracket 1 \pm 2[p^2 + (|r| + |2u \sin 2\varphi - r \cos 2\varphi|)^2]^{1/2} \rrbracket. \quad (24)$$

In Eqs. (22) and (23), S and S_r are the entropies of the full and reduced density matrices, respectively:

$$S = - \sum_{j=1}^4 \lambda_j \log_2 \lambda_j, \quad (25)$$

where the eigenvalues λ_j of the density matrix under consideration are given as

$$\lambda_{1,2} = \frac{1}{4} + q \pm [p^2 + (2u \sin 2\varphi - r \cos 2\varphi)^2]^{1/2}, \quad \lambda_{3,4} = \frac{1}{4} - q \pm |r|, \quad (26)$$

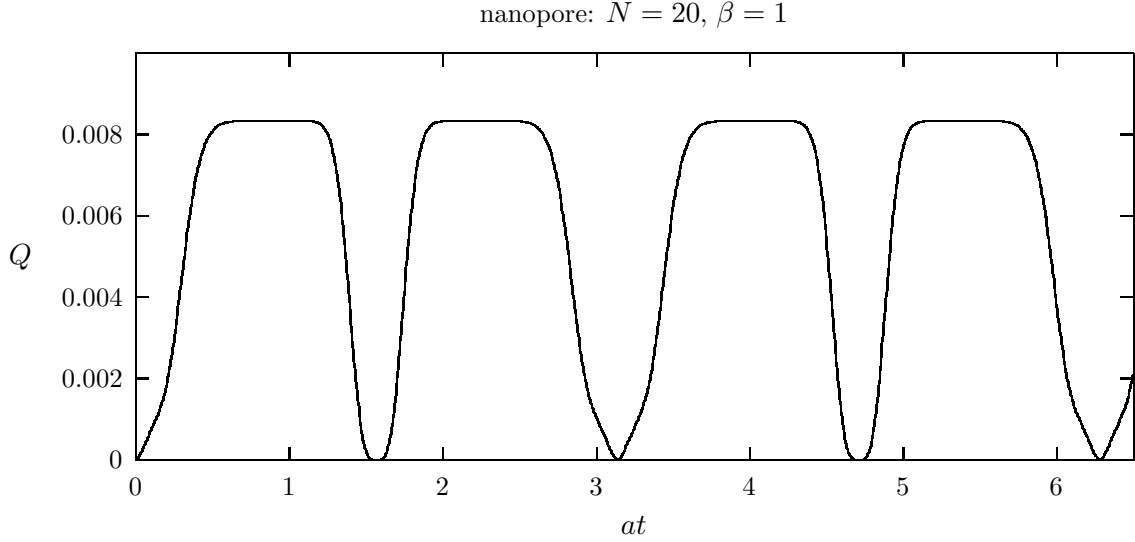


FIG. 1: Quantum discord in nanopore as a function of dimensionless time.

and

$$S_r = -\left(\frac{1}{2} + p\right) \log_2\left(\frac{1}{2} + p\right) - \left(\frac{1}{2} - p\right) \log_2\left(\frac{1}{2} - p\right). \quad (27)$$

Typical time dependence for the pairwise quantum correlation of spin-carrying particles in a nanopore is shown in Fig. 1. The correlation oscillates between zero and the saturation value which is Q when $p = u = 0$ and $r = q = \frac{1}{8} \tanh^2(\beta/2)$ [see Eq. (26) in Ref. 7].

Our third example concerns with the pseudopure (PP) states

$$\rho_{PP} = \alpha |\psi\rangle\langle\psi| + \frac{1-\alpha}{4} I, \quad (28)$$

where $|\psi\rangle$ is an arbitrary two-qubit pure state, I is the identity operator, and the probability $\alpha \in [0, 1]$. The states like (28) are studied as a possible resource for NMR quantum computing (see, e. g., [9] and references therein). It is easy to check that if

$$|\psi\rangle = a(|00\rangle + |11\rangle) + b(|01\rangle + |10\rangle) \quad (29)$$

($|a|^2 + |b|^2 = 1/2$ and $\{|00\rangle, |01\rangle, |10\rangle, |11\rangle\}$ is the computational basis) the state ρ_{PP} will be CS one and we can calculate its quantum discord using the above scheme.

Conclusions. We have established the relation between the CS and X matrices via the universal local orthogonal transformation. This allows to find the discord of any CS states using available formulas for the discord of X states. CS quantum states appear in different important physical problems, three of which have been discussed.

This work was supported by the RFBR (project No. 13-03-00017).

- [1] K. Modi, A. Brodutch, H. Cable, T. Paterik, and V. Vedral, *Rev. Mod. Phys.* **84**, 1655 (2012).
- [2] T. Yu and J. H. Eberly, *Quantum Inf. Comput.* **7**, 459 (2007).
- [3] A. R. P. Rau, *J. Phys. A: Math. Theor.* **42**, 0412002 (2009).
- [4] M. Ali, A. R. P. Rau, and G. Alber, *Phys. Rev. A* **81**, 042105, (2010); **82**, 069902(E) (2010);
B.-F. Ding, X.-Y. Wang, and H.-P. Zhao, *Chin. Phys. B* **20**, 100302 (2011); Q. Chen, C. Zhang,
S. Yu, X. X. Yi, and C. H. Oh, *Phys. Rev. A* **84**, 042313 (2011).
- [5] J. R. Weaver, *Am. Math. Mon.* **92**, 711 (1985); A. Andrew, *SIAM Rev.* **40**, 697 (1998).
- [6] Y.-X. Chen and Y. Zhi, *Commun. Theor. Phys.* **54**, 02536102 (2010).
- [7] E. B. Fel'dman, E. I. Kuznetsova, and M. A. Yurishchev, *J. Phys. A: Math. Theor.* **45**, 475304
(2012).
- [8] F. F. Fanchini, T. Werlang, C. A. Brasil, L. G. E. Arruda, and A. O. Caldeira, *Phys. Rev. A*
81, 052107 (2010); B. Li, Z.-X. Wang, and S.-M. Fei, *Phys. Rev. A* **83**, 022321 (2011).
- [9] J. Maziero, R. Auccaise, L. C. Céleri, D. O. Soares-Pinto, E. R. deAzevedo, T. J. Bonagamba,
R. S. Sarthour, I. S. Oliveira, and R. M. Serra, arXiv: 1212.2427 [quant-ph].